Takahashi Integral Equation and High-Temperature Expansion of the Heisenberg Chain

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(Dated:)

Recently a new integral equation describing the thermodynamics of the 1D Heisenberg model was discovered by Takahashi. Using the integral equation we have succeeded in obtaining the high temperature expansion of the specific heat and the magnetic susceptibility up to $O((J/T)^{100})$. This is much higher than those obtained so far by the standard methods such as the linked-cluster algorithm. Our results will be useful to examine various approximation methods to extrapolate the high temperature expansion to the low temperature region.

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The spin-1/2 Heisenberg chain is the one of the fundamental models which has been continuously investigated in the realm of the magnetism in low dimensions. In 1931, Bethe constructed the eigenstates for the isotropic case [1], which was later generalized to anisotropic cases such as the XXZ and the XYZ chain (see [2]). The method, which is nowadays called Bethe ansatz method, has provided us vast information on the model. Especially the thermodynamics has been studied through the Thermodynamic Bethe Ansatz (TBA) equations [2, 3, 4, 5, 6, 7] and the Quantum Transfer Matrix method (QTM) [8, 9, 10, 11, 12, 13, 14, 15, 16].

Quite recently, one of the authors (MT) has found yet another integral equation [17], which determines the free-energy of the XXZ chain. The integral equation consists of one unknown function and is very simple. We have found that it actually gives the same numerical values for physical quantities as those calculated by the TBA equations and the QTM method. In fact the equation was originally discovered in an attempt to simplify the TBA equations [17]. Soon after that it was derived also from the fusion relation of the QTM [18].

In this letter, as one of the applications of this integral equation, we study the high temperature expansion (HTE). As is well known, there is a systematic way to calculate the HTE for any lattice models based on the linked-cluster algorithm [19, 20]. Particularly, in the case of the XXX chain, the HTE has been achieved up to $O((J/T)^{24})$ [20]. We have succeeded in obtaining the HTE to much higher order, namely, up to $O((J/T)^{100})$ by use of the new integral equation. Below we shall report the result for the isotropic XXX model. The generalization to the anisotropic models will be published in a separate paper.

The Hamiltonian of the spin-1/2 Heisenberg XXX chain is defined by

$$
\begin{aligned}
H = &-J\sum_{j=1}^{N}\left[S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+S_j^zS_{j+1}^z-\frac{1}{4}\right] \\
&-2h\sum_{j=1}^{N}S_i^z,
\end{aligned}
\tag{1}
$$

where $S_j^{x,y,z}$ are the local spin-1/2 operators acting on the site j.We assume the periodic boundary conditions $S_{N+1}=S_1$. Note that in our definition, the coupling constant J is positive for the ferromagnetic case and negative for the antiferromagnetic case.

Takahashi's integral equation for the isotropic XXX case is given by

$$
\begin{aligned}
u(x) &= 2\cosh h/T \\
&\quad+\oint_C\left\{\frac{1}{x-y-2\mathrm{i}}\exp\left[-\frac{2J/T}{(y+\mathrm{i})^2+1}\right]\right. \\
&\quad\left.+\frac{1}{x-y+2\mathrm{i}}\exp\left[-\frac{2J/T}{(y-\mathrm{i})^2+1}\right]\right\}\frac{1}{u(y)}\frac{\mathrm{d}y}{2\pi\mathrm{i}}, \\
f &= -T\ln u(0),
\end{aligned}
\tag{2}
$$

where the contour C is a loop surrounding the origin in a counterclockwise manner. The equation can be solved numerically.

In the following we derive the HTE of $u(x)$. Actually what we have to do is only to assume $u(x)$ in the form

$$
\begin{aligned}
u(x) &= \exp\left[\sum_{n=0}^{\infty}a_n(x)\,(J/T)^n\right] \\
&= \mathrm{e}^{a_0(x)}\left\{1+a_1(x)J/T+\left(a_2(x)+\frac{1}{2}a_1(x)^2\right)(J/T)^2\right. \\
&\quad\left.+\left(a_3(x)+a_2(x)a_1(x)+\frac{1}{6}a_1(x)^3\right)(J/T)^3+\cdots\right\}.
\end{aligned}
\tag{3}
$$

and substitute it into the equation (2). Then by comparing the same order of J/T in the LHS and the RHS, we can get the equations, which, to our surprise, determine the functions $a_n(x)$ recursively. For example, from the 0-th order, we get immediately

$$a_0(x) = \ln\left(2\cosh h/T\right). \tag{4}$$

Similarly by comparing the 1-st order, we have an equation,

$$\begin{aligned} a_1(x) \;=\; & \frac{1}{4\cosh^2 h/T}\Bigg[\oint_C \left\{\frac{-2}{y(y+2\mathrm{i})(x-y-2\mathrm{i})}\right. \\ & \qquad\left. +\frac{-2}{y(y-2\mathrm{i})(x-y+2\mathrm{i})}\right\}\frac{\mathrm{d}y}{2\pi\mathrm{i}} \\ & -\oint_C \left\{\frac{1}{x-y-2\mathrm{i}}+\frac{1}{x-y+2\mathrm{i}}\right\}a_1(y)\frac{\mathrm{d}y}{2\pi\mathrm{i}}\Bigg]. \end{aligned} \tag{5}$$

Noting that the second term in the RHS vanishes because the integrand is regular at $y=0$, we can calculate $a_1(x)$ explicitly as

$$a_1(x) = -\frac{1}{\cosh^2 h/T}\frac{1}{x^2+4}. \tag{6}$$

Repeating the similar procedures we can derive each $a_n(x)$ successively. For example, we have found

$$\begin{aligned} a_2(x) \;=\; & \frac{1}{4\cosh^2 h/T}\frac{x^2+12}{(x^2+4)^2} \\ & -\frac{1}{4\cosh^4 h/T}\frac{x^2+6}{(x^2+4)^2}, \end{aligned} \tag{7}$$

$$\begin{aligned} a_3(x) \;=\; & -\frac{1}{24\cosh^2 h/T}\frac{3x^4+36x^2+160}{(x^2+4)^3} \\ & +\frac{1}{4\cosh^4 h/T}\frac{x^4+11x^2+36}{(x^2+4)^3} \\ & -\frac{1}{24\cosh^6 h/T}\frac{3x^4+30x^2+80}{(x^2+4)^3}. \end{aligned} \tag{8}$$

In fact, with the help of *Mathematica*, we have calculated $a_n(x)$ up to $n=100$, which provides the HTE for the free energy $f/T = -\sum_{n=0}^{\infty} a_n(0)(J/T)^n$ up to $(J/T)^{100}$. Some of the lower terms are given as

$$\begin{aligned} f/T = & -\ln(2\cosh(h/T)) + \frac{J}{4T}(1-B^2) \\ & -\frac{3J^2}{32T^2}\left(1-B^4\right) \\ & +\frac{J^3}{192T^3}(1-B^2)(3+7B^2+10B^4) \\ & +\frac{5J^4}{3072T^4}(1-B^2)(3-B^2-9B^4-21B^6) \\ & -\frac{J^5}{5120T^5}(1-B^2)(1+2B^2) \\ & \qquad\times(15-B^2+21B^4-63B^6) \\ & -\frac{7J^6}{122880T^6}(1-B^2) \\ & \times(3-35B^2-85B^4-95B^6-30B^8+330B^{10}) \\ & +\ldots, \end{aligned} \tag{9}$$

where we have set $B=\tanh(h/T)$. From the expansion (9), one can get the HTE for other physical quantities.

For example, we list coefficients of the HTE for the specific heat $C = -T\frac{\partial^2 f}{\partial T^2}$ and the magnetic susceptibility $\chi = -\frac{\partial^2 f}{\partial h^2}$ at zero magnetic field in Table I and Table II. Unfortunately due to the lack of space, we can present the coefficients only up to $O((J/T)^{51})$. The coefficients of higer order will be sent on demand to any interested reader. We remark that the coefficients up to $O((J/T)^{24})$ completely coincide with those given in [20].(Note the differences of the conventions, $J \leftrightarrow -J$ and $h \leftrightarrow 2h$.) The terms with the order larger than $O((J/T)^{25})$ are our new results. It will probably be impossible to get the HTE to such a high order using a conventional method.

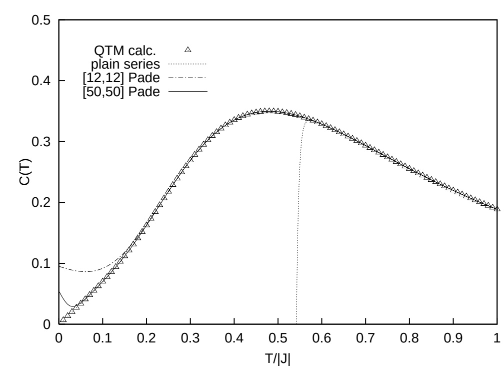

FIG. 1: Specific heat for the antiferromagnetic XXX chain at $h=0$.

Usually in order to extrapolate the high temperature expansion series to the low temperature region, some further approximation methods are used. Actually the original series will not converge in the low temperature region (T about less than 0.55), because of the existence of the singularities on the complex plane with respect to the inverse temperature.

Here we have applied the standard Padé approximation to our HTE. The results are shown in Fig. 1,...,Fig. 4.

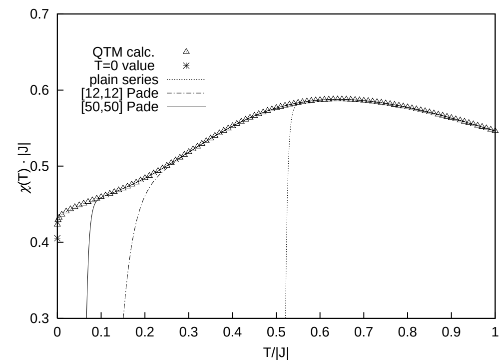

FIG. 2: Magnetic susceptibility for the antiferromagnetic XXX chain at $h = 0$. $\chi(0)$ is taken from [21].

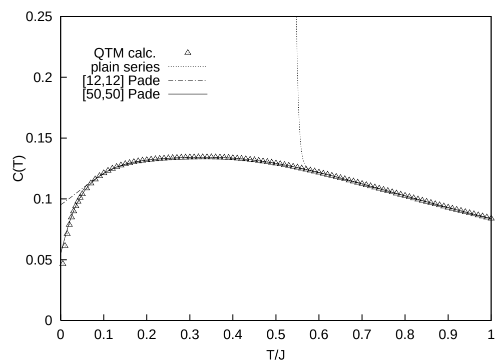

FIG. 3: Specific heat for the ferromagnetic XXX chain at $h = 0$.

Since we have obtained the HTE up to $O((J/T)^{100})$, the expressions up to $[50, 50]$ Padé approximant are available. For comparison, we have also plotted the numerical data calculated by the QTM method [11, 15]. (Note that the physical quantities in Fig. 1,...,Fig. 4 were first calculated by the TBA equations. See particularly [6, 7] for the ferromagnetic case.) From Fig. 1,...,Fig. 4, we find that the $[50, 50]$ Padé approximant show good coincidence with data by the QTM to very low temperature region somewhat like $T \sim 0.05$ except for the the magnetic susceptibility for the antiferromagnetic case (Fig. 2.). In that case the logarithmic anomaly around $T \to 0$ is so strong [14, 15, 16] and it probably prevents the good convergence of the Padé approximation [20].

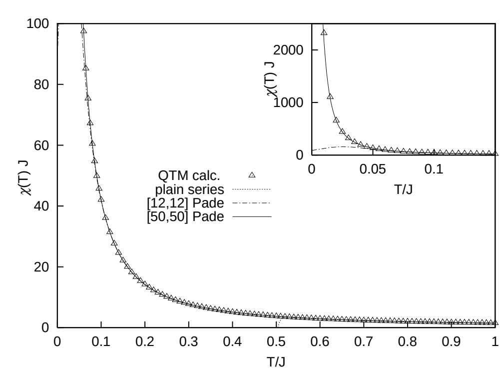

FIG. 4: Magnetic susceptibility for the ferromagnetic XXX chain at $h = 0$. Note that the plain series of HTE deviates from the QTM data around $T = 0.52$.

Apart from the very low temperature region, we have found our higher order Padé approximation gives the physical quantities with extremely high precision. For example, we have estimated the peak position of the specific heat and the magnetic susceptibility for the antiferromagnetic case by use of our $[50, 50]$ Padé approximation. The result for the specific heat is

$$\begin{aligned} C^{\max} &= 0.3497121234553176, \\ T^{\max}/|J| &= 0.4802848685890477, \end{aligned} \tag{10}$$

and that for magnetic susceptibility is

$$\begin{aligned} \chi^{\max}|J| &= 0.5877051177413559, \\ T^{\max}/|J| &= 0.6408510308513831. \end{aligned} \tag{11}$$

These values are perfectly identical to the ones in [16], where the non-linear integral equations for the QTM were solved numerically very carefully. (Note that our $\chi^{\max}|J|$ is four times larger than that in [16], because of different normalization factors.) Note also that the peak position of the magnetic susceptibility (11) was first determined in [14].

For comparison we have also estimated the peak position of the specific heat for the ferromagnetic case as

$$\begin{aligned} C^{\max} &= 0.1342441913136996, \\ T^{\max}/J &= 0.3326119630964252. \end{aligned} \tag{12}$$

In conclusion, we have shown that the the new integral equation by Takahashi is very useful to calculate analytically the HTE for the 1D Heisenberg model. As far as we know, the HTE of such a high order as $O((T/J)^{100})$ has not been achieved for any other models except for free ones. We have seen that our HTE data together with Padé approximation, provide the very accurate numerical data for physical quantities to sufficiently low temperatures. There are several further methods to improve the Padé approximation, for example, to allow for the asymptotic expression as $T \to 0$, etc. (see, for example, [20, 22]). Based on the present results we shall investigate such possibilities in the forthcoming publication.

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TABLE I: Series coefficients α_n for the high temperature expansion of the specific heat $C = \sum_n \frac{\alpha_n}{n!} \left(\frac{J}{4T}\right)^n$ at $h = 0$.

n	α_n	n	α_n
0	0	26	484455914465376683487755420408217600
1	0	27	-1592964364128699671723658807556964352
2	6	28	-16592223413777236744548930659363711877 12
3	-36	29	53827694891210973745020673240061454581760
4	-360	30	5090517962961447184851808942927438864711680
5	7200	31	-388446833192725659973817494776649147157053440
6	15120	32	-11028658525378274359384407389662010654796546048
7	-1848672	33	2255854109806569120380670028755308714386167693312
8	11426688	34	-188787025806229890700787934823639934257018070630 40
9	594846720	35	-11721570087037734701356860480896473609272542720163840
10	-11558004480	36	527183038642469386328859769728396518893185382125404160
11	-199812856320	37	52548749252010967993948480669499712309299856992951599104
12	10106191180800	38	-5382365237582398925074954773487741035075672601159589167104
13	19376365252608	39	-150281021589219619860159284209265140804955107276364175114240
14	-9289795522775040	40	44482678475307391762958213932359681737961800852665438128046080
15	121944211136778240	41	-670778300712303276022754187872671936481343744506621812675706880
16	879178139011694592 0	42	-3233111851262535303334911142992092649497388429937499549362387156992
17	-310402124957945954304	43	19271391500067613736198673193545354611765664770995927250862568636416
18	-7225535925744106143744	44	1963797073102024140530884388201619017857423297479642613447074848440320
19	643407197363813620776960	45	-261757449501391383349154989821467694962901907072496780634929173522022400
20	96147483542540314214400	46	-6715036186134671522475926929150627328836680429076585020863949295740518400
21	-1279121513829538179364945920	47	2897640509780835688484069216581936412870887902144153768250804439297575354368
22	27962069861743501862336200704	48	-678845838424482527057294933805899162845435905920892435456258166630556840755 20
23	2398518627113966015427501883392	49	-27839667354545349510646207322267839343449407617219100508752156300912706663 2192 00
24	-129834725539335848980192847462400	50	2130333568970965233678580974509426707048585535358286474483865352948915543579033600
25	-3493877000064415911285457158144000	51	216827879657653769500650387534438914339017251205042192428944 424756474567924803174400

TABLE II: Series coefficients β_n for the high temperature expansion of the magnetic susceptibility $\chi = \frac{1}{T} \sum_n \frac{\beta_n}{(n+1)!} \left(\frac{J}{4T}\right)^n$ at $h = 0$.

n	β_n	n	β_n
0	1	26	108250895627317866042581831619969024
1	4	27	-17922781862082598948422103131404369920
2	0	28	120323704775766862241382488276073447424
3	-64	29	6372649919697951163441811694039418798080 0
4	400	30	-2379574083879736929901931437077028466065408
5	4032	31	-199921736549129208105099470038165104315334656
6	-89376	32	17205669691857844357030111005301702510893858816
7	-163840	33	408607241970908762765181373729511748361273737216
8	26313984	34	-102465082506734431652137262962322034251260126822400
9	-191334400	35	1315775281576476974395821022113890916515475892469760
10	-9565698560	36	545540112377157932817560176143490374271324160383778816
11	210597986304	37	-27991080178083294022121824180738137056773157996564840448
12	3486950684672	38	-2463499970265937469283180992880401729855043417164218368000
13	-203634731188224	39	284868319106208295442521316317947214008165828662443533926400
14	-127324657152000	40	6335450833027827824904755798342667046011674072210769010753536
15	205019990184689664	41	-239325639117088753477381102348233554857599390577124798906341 7856
16	-3169755454477500416	42	49322825714830688230041284007303368927055837926052566121716908032
17	-208763541109969256448	43	1765580916346232017964366104109992358215628089928865922947044972953 6
18	8342101010835559022592	44	-1192343745774700569487973174622411288186826884326738448519272595456000
19	175912858271144581529600	45	-106665300086792728016396630723577790891277245485607114802374328230871040
20	-18366266410738921187573760	46	16097399250631032968718675605919227751757635356066434920608362971107688448
21	407803172892468728509235 20	47	306091410138596910653186173722480725145635803390769178021236250893761904640
22	38668138493195891009425244160	48	-18002201464771464928560915719667347918570756248339001237500236247953 6 725032960
23	-983734184997038611238624428032	49	5408449632892687473365326165267541130523650154708192975684794827854640578560000
24	-75650797544886562610211717120000	50	17426550003663298365992833617318506452913828517681 694079865166325697655461013 09440
25	4622511990582180728868776781545472	51	150302197636602238677940274995321497800768163734200678571365174132101 0 78803395117056

[1] H. A. Bethe, Z. Phys. **71** 205 (1931).

[2] M. Takahashi, Thermodynamics of One-Dimensional Solvable Models, (Cambridge University Press, Cambridge, 1999)

[3] M. Takahashi, Prog. Theor. Phys. **46**, 401 (1971).

[4] M. Gaudin, Phys. Rev. Lett. **26**, 1301 (1971).

[5] M. Takahashi and M. Suzuki, Prog. Theor. Phys. **46**, 2187 (1972).

[6] M. Takahashi and M. Yamada, J. Phys. Soc. Jpn. **54**, 2808 (1985).

[7] P. Schlottmann, Phys. Rev. Lett. **54**, 2131 (1985).

[8] M. Suzuki and M. Inoue, Prog. Theor. Phys. **78**, 787 (1987).

[9] T. Koma, Prog. Theor. Phys. **78**, 1213 (1987); *ibid* **81**, 783 (1989).

[10] J. Suzuki, Y. Akutsu, and M. Wadati, J. Phys. Soc. Jpn. **59**, 2667 (1990).

[11] M. Takahashi, Phys. Rev. B **43**, 5788 (1991) ; *ibid* **44**,

12382 (1991).
[12] M. Takahashi *et al.*, Phys. Rev. Lett. **67**, 746 (1991).
[13] A. Klümper, Z. Phys. B **91**, 507 (1993).
[14] S. Eggert, I. Affleck, and M. Takahashi, Phys. Rev. Lett. **73**, 332 (1994).
[15] A. Klümper, Eur. Phys. J. B **5**, 677 (1998).
[16] A. Klümper and D. C. Johnston, Phys. Rev. Lett. **84**, 4701 (2000).
[17] M. Takahashi, in *Physics and Combinatrics*, eds. A. K. Kirillov and N. Liskova, P299-304, (World Scientific, Singapore, 2001), cond-mat/0010486.
[18] M. Takahashi, M. Shiroishi, and A. Klümper, J. Phys. A. Math. Gen. **34**, L187 (2001).
[19] G. A. Baker, G. S. Rushbrooke, H. E. Gilbert, Phys. Rev. **135**, A1272 (1964).
[20] A. Bühler, N. Elstner, and G. S. Uhrig, Eur. Phys. J. B **16**, 475 (2000).
[21] R. B. Griffiths, Phys. Rev. **133**, A768 (1964).
[22] A. Bühler, U. Löw, and G. S. Uhrig, Phys. Rev. B **64**, 024428 (2001).